D1.2 – Summer school

BeforeHand – 824957

Covering the reporting period from
01/01/2019 to 28/02/2022
Reporting Date
28/02/2022

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Project website: www.beforehand.eu

Horizon 2020 work programme within the Objective ICT-07-2018: Electronic Smart Systems (ESS)

Summary

1 Introduction

The present document is a Deliverable generated by the WP1 "Management" and it is focused on a report on the realization of the BeforeHand school 2022 on phase change materials. The date of submission of such deliverable after the last project amendment was due on 30th of September 2021, as it should occur in person after the E/PCOS2021. However, the E/PCOS 2021 was held in virtual format and thus we decided to wait till the beginning of 2022 to have a large percentage of European citizen vaccinated against Covid-19. Such delay was approved by the Project Officer at the technical review meeting in July 2021. Surprisingly, the Omicron mutation of the Covid-19 virus stimulated a strong wave of infections right after Christmas 2021, therefore we decided that to fulfil such deliverable we would better organise the School in a virtual format, instead of risking no participation due to infections and Covid restrictions.

2 BeforeHand 2022 School of Phase Change Materials

The BeforeHand 2022 School of Phase Change Materials took place on the 23rd and 24th of February 2022 online.

The School was organized by Dr. R. Calarco from partner CNR-IMM and coordinator of BeforeHand and by Prof. Dr. Fabrizio Arciprete from the partner University of Rome "Tor Vergata".

The School was embedded in the program of Materials Science and Technology Master Degree of the University of Rome "Tor Vergata", for which the undergraduate students obtained 1 University Formative Credit (within the European Credit Transfer and Accumulation System - ECTS). The BeforeHand School covered the fields of phase change materials physics and related advanced technologies. The BeforeHand School's distinguishing feature was the joint contribution of young and expert physicists and engineers on the phase change material topics centred around the BeforeHand Project. This concept builds on - and in turn strengthens - the key feature of the BeforeHand Project, which combines the vivid academic environment of universities with the "big science" infrastructure of national research centres and the applicative industrial environment. An important characteristic of the BeforeHand School was the European environment that originates from our collaborations. The leitmotif of the BeforeHand School was the optimal training on a very specific topic of young students and researchers for careers in science and industry through participation at such School organized within an international project. The School was open not only to undergraduate students from the Materials Science and Technology Program of the University of Rome "Tor Vergata", but also to graduate, Ph.D and postdoctoral researchers. Such participants were mainly related to the BeforeHand partners. However, the School was open to external participants as well.

The School Program is reported in the following table:

Wednesday February 23rd 2022	
09:00 – 09:15	**Opening** by: Raffaella Calarco **– CNR-IMM Roma**
09:15 – 10:00	**Lecture 1** **Title: Introduction to phase change materials (PCM)** **by: Bart Kooi – University of Groningen**
10:00 – 10:15	**Break**
10:15 – 11:00	**Lecture 2** **Title: PCM electrical memories** **by: Andrea Redaelli – STMicroelectronics Agrate Brianza**
11:00 – 11:15	**Break**
11:15 – 12:00	**Lecture 3** **Title: Neuromorphic computing** **by: Valeria Bragaglia IBM Zuerich**
12:00 – 12:15	**Break**
12:15 – 13:00	**Lecture 4** **Title: PCM material synthesis and fabrication** **by: Massimo Longo – CNR-IMM Roma**

Thursday February 24th 2022	
09:00 – 09:15	**Opening** By: Raffaella Calarco **– CNR-IMM Roma**
09:15 – 10:00	**Lecture 5** **Title: Introduction to PCM theoretical calculations by: Riccardo Mazzarello – La Sapienza Università di Roma**
10:00 – 10:15	**Break**

10:15 – 11:00	**Lecture 6** **Title: PCM thermal properties - Theory** **by: Marco Bernasconi – Università di Milano Bicocca**
11:00 – 11:15	**Break**
11:15 – 12:00	**Lecture 7** **Title: PCM thermal properties - Experiment** **by: Jean-Luc Battaglia – CNRS I2M University of Bordeaux**
12:00 – 12:15	**Break**
12:15 – 13:00	**Lecture 8** **Title: PCM structural investigations** **by: Antonio Mio – CNR-IMM Catania**

Our means of teaching were online block lectures, which were very time-efficient and well suited to undergraduate students during the semester free time. In overall we had 8 lectures. We privileged the participation of lecturers form the BeforeHand consortium also to enhance the consortium visibility. However, we managed to attract two excellent external lecturers (25% of the speakers): Prof. Riccardo Mazzarello (Sapienza University of Rome) expert in Molecular Dynamics of Phase Change Materials and Dr. Valeria Bragaglia working on Neuromorphic architectures at IBM Zuerich.

3 Lecture Abstracts

In the following we present the abstracts of the lectures given during the School to specify the topics presented by each lecturer. Some of the slides presented at the School were made available upon request to the students. Those documents were intended only for private use no commercial use was allowed. The students did not receive the permission to publish or put the slides in internet or provide them to others.

Lecture 1

Introduction to phase change materials (PCM)

Bart J. Kooi

Zernike Institute for Advanced Materials, University of Groningen, The Netherlands

Phase change materials (PCMs) exhibit a unique combination of properties till date only found in a limited range of materials generally containing antimony and/or tellurium. This introductory lecture particularly focuses on structure, properties and applications of PCMs. The distinction is made between nucleation and growth dominant materials. The special crystallization kinetics, including the role played by fragility, is highlighted e.g. the amorphous phase is stable for 10 years at 80 °C, while it still can crystallize within 100 ns at 500 °C. In amorphous PCMs covalent bonding prevails, but the crystalline PCMs exhibit a special type of bonding that has been coined metavalent bonding. Crystal structures are peculiar with general octahedral coordination which easily show Peierls distortion with 3 stronger and 3 weaker bonds. Also high concentrations of structural vacancies can be present which can play an important role in the insulator to metal transition. After the introduction of basic structures and properties, the applications of PCMs in optical recording, switchable metamaterials, RAM based memories and neuromorphic computing are shortly explained. For neuromorphic computing resistance drift of the amorphous phase requires prime attention and two methods to supress it are shown.

Lecture 2

Phase Change Memory physics and technology

Andrea Redaelli

STMicroelectronics, Agrate Brianza, Italy

The lecture will start by introducing the Phase Change Memory (PCM) concept. The basic PCM operation will be then reviewed highlighting the main opportunities of this device in terms of performance and reliability comparing it with actual mainstream memories. The novel physics underneath PCM operation is discussed with special attention to amorphous conduction and phase change description. Concerning the possible applications, two possible paths of interest are identified for PCM. PCM for standalone applications required a strong device and process engineering efforts to provide high density and low-cost memories that ended up with the 3DXpoint memory. On the other hand, PCM for embedded applications required a strong material engineering effort, offering much high reliability suitable for more demanding System on Chip (SoC) markets. Recent results of actual PCM-based products are discussed, suggesting a brilliant future for chalcogenide-based solid-state memories.

Lecture 3

Materials for Neuromorphic Computing: Overcoming the Von-Neumann Bottleneck

Valeria Bragaglia

IBM Zurich GmbH

In this lecture I will introduce the concept of neuromorphic computing, highlighting why it is a promising approach for the post non Von-Neumann computing era.

Why is our brain so outstanding and why do we want to mimic it? The answer is found by looking at what AI workloads are, and by understanding how deep artificial neural networks (ANN) come into play. Nonetheless, solving AI tasks on today's computers is heavily time inefficient due to the data bus between the physically separated processing and memory units. This concept is known as Von-Neumann bottleneck.

In the neuromorphic computing paradigm, a promising solution are crossbar arrays of non-volatile analogue memories, also known as memristors. In this architecture the physical separation between memory and processing unit is closed, allowing to implement operation with ANN at potential O(1) time complexity.

Lecture 4

PCM material synthesis and fabrication

Massimo Longo

CNR-IMM Rome, Italy

The realization of nonvolatile memory devices based on Phase Change Materials (PCM) starts from their synthesis, which can be achieved using different advanced deposition methods.
To realize active materials that, suitably processed, respond to the continuous need of obtaining increasingly highly performing devices, it is, therefore, necessary to select the best growth methods and the most appropriate deposition conditions. This lesson aims to provide an overview of the most popular methods for the realization of PCM materials, from the basic principles to their applications to specific cases, with a focus on the most studied Ge-Sb-Te alloys, either in the form of thin films, or multilayered heterostructures, or nanowires.

After introducing the materials of interest and the concepts of growth, fabrication, and nanoscaling, both physical (such as sputtering, MBE, PLD) and chemical (such as CVD, MOCVD, ALD) methods for the synthesis of PCM materials for memory devices will be illustrated; finally, some conclusions on the criteria for their choice will be drawn.

Lecture 5

Introduction to PCM theoretical calculations

Riccardo Mazzarello

La Sapienza Università di Roma, Italy

Phase-change materials (PCMs) are used in optical devices and electronic non-volatile memories, and are promising candidates for neuro-inspired computing applications. These technologies exploit the ability of PCMs to switch rapidly between amorphous and crystalline states with pronounced optical and electrical contrast. In this tutorial an overview is given of recent computational work on PCMs based on density functional theory. It will be shown that simulations have enabled the elucidation of fundamental

links between structure and dynamics. Such links have shed light on technologically relevant properties of PCMs, including the ultrafast crystallization at high temperature, the behaviour of the liquid phase in the deep undercooling regime and the relaxation of the amorphous state.

Lecture 6

PCM thermal properties – Theory

Marco Bernasconi

Department of Materials Science, University of Milano-Bicocca, Milano, Italy

Chalcogenide materials such as the GeSbTe (GST) alloys are of interest for applications in non-volatile phase change memories (PCM) thanks to their ability to undergo a fast and reversible transformation between the crystalline and amorphous phase upon Joule heating. Thermal conductivity is a key factor for the device operation, as the set/reset processes strongly depend upon heat dissipation and transport. The thermal boundary resistance at the interface between the phase change material and the surrounding dielectrics or metallic electrodes is another crucial parameter for the control of thermal cross-talks between adjacent cells which may arise during memory programming. A large boundary resistance can also lead to a reduction in the programming current thanks to heat confinement effects.

In this lecture, I will briefly review theoretical results on the simulation of thermal transport in the crystalline and amorphous phase of chalcogenide alloys for PCM. Methods based on the solution of Boltzmann transport equation for phonons based on density functional theory (DFT) and large scale non-equilibrium molecular dynamics simulations employing machine learning interatomic potentials will be briefly discussed.

The calculation of the different contribution to thermal boundary resistance of GST alloys and of the parent GeTe compound with prototypical metallic electrodes, including electron-phonon coupling, will also be discussed.

Lecture 7

Measuring the thermal properties of phase change materials (PCM): From the PCM to the PCRAM

Jean-Luc Battaglia

I2M-CNRS, University of Bordeaux, France

The course will start with an illustration of the importance of the thermal properties of the PCMs from the simulation of the RESET within a PCRAM device, considering the “mushroom” and “nanowire” configurations. In a second step, the different contact and contact less methods used to estimate those thermal properties will be presented. Each method is assumed to lead to complementarity information with others and some are also more suited for high-temperature characterization where the phase change is

expected to occur. The third part of the course is devoted to the implementation of invers methods. Indeed, for all the presented techniques, the thermal parameters are identified from the measurements and a model of the experiment. The parameters are therefore identified by minimizing the gap between both quantities. Finally, two illustrations are given that show the advantages and the limits for all the proposed experimental techniques.

Lecture 8

PCM structural investigations by Transmission Electron Microscopy

Antonio Massimiliano Mio

Institute for Microelectronics and Microsystems (IMM), Consiglio Nazionale delle Ricerche (CNR), Italy

Phase-Change Materials (PCMs), mainly represented by GeTe-Sb2Te3 (GST) alloys, are used since the 80s for high-density data storage in optical media. Lately, the use of these alloys has been extended to solid-state non-volatile memories. These applications of PCMs rely on very fast (<100ns) phase transitions and on the pronounced optical and resistive contrast between the amorphous and crystalline state. Recently it has been shown that multi-layered crystalline phase change materials, arranged in superlattice and/or high-ordered systems, can exhibit improved functional properties.

Additionally, the development of PCMs for novel applications (e.g. multi-level memories, neuromorphic devices, thermoelectrics, …) requires a precise control of the nanoscale inhomogeneities (i.e. phase separations, defects, grain boundaries, precipitates) that must be engineered or avoided.

With the aim of a better insight into the local structural arrangement of PCMs, we discuss about nanoscale studies performed by means of conventional Transmission Electron Microscopy, High Angular Annular Dark Field (HAADF) Scanning/TEM (S/TEM) and correlated nano-analysis techniques.

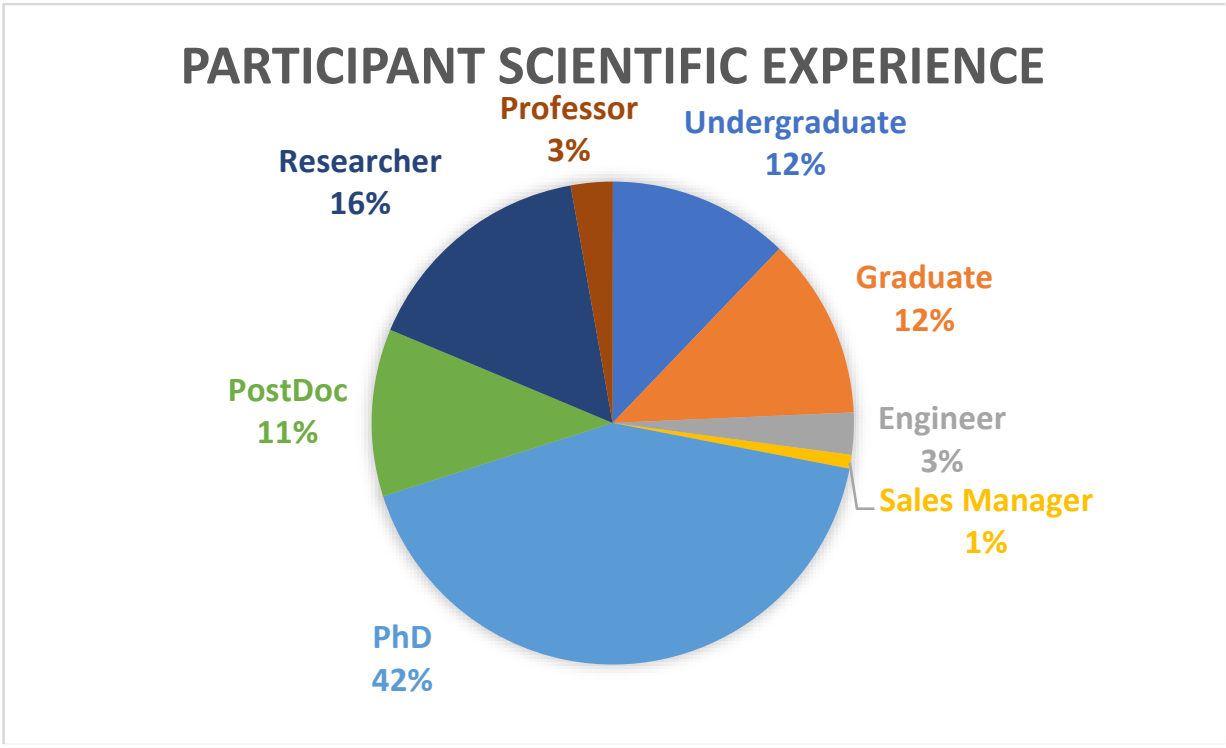
HAADF STEM directly relates the micrograph contrast to the atomic number (Z-contrast), permitting a straightforward interpretation of the images. Therefore in GST, where planes of Te only (anions) alternate plane of Ge/Sb/vacancy (cations), high-intensity Te planes and lower intensity Ge/Sb/vacancy layers can be directly identified. Van der Waals gaps formation and differences in cation-anion plane distance, related to the bonding between these two layers, can be observed in several transition steps. This also allows a straightforward inspection of the vacancy ordering dynamics, related to the conversion into the stable trigonal phase, for different morphology of the initial rock-salt phase (metastable). As a result, according to the substrate and to the crystallization path, we can distinguish upon resistance values characterized by different degree of structural order, necessary for the development of multi-level phase change data storage.

4 Attendees

We achieved an overall number of 110 attendees with the following scientific background characteristics:

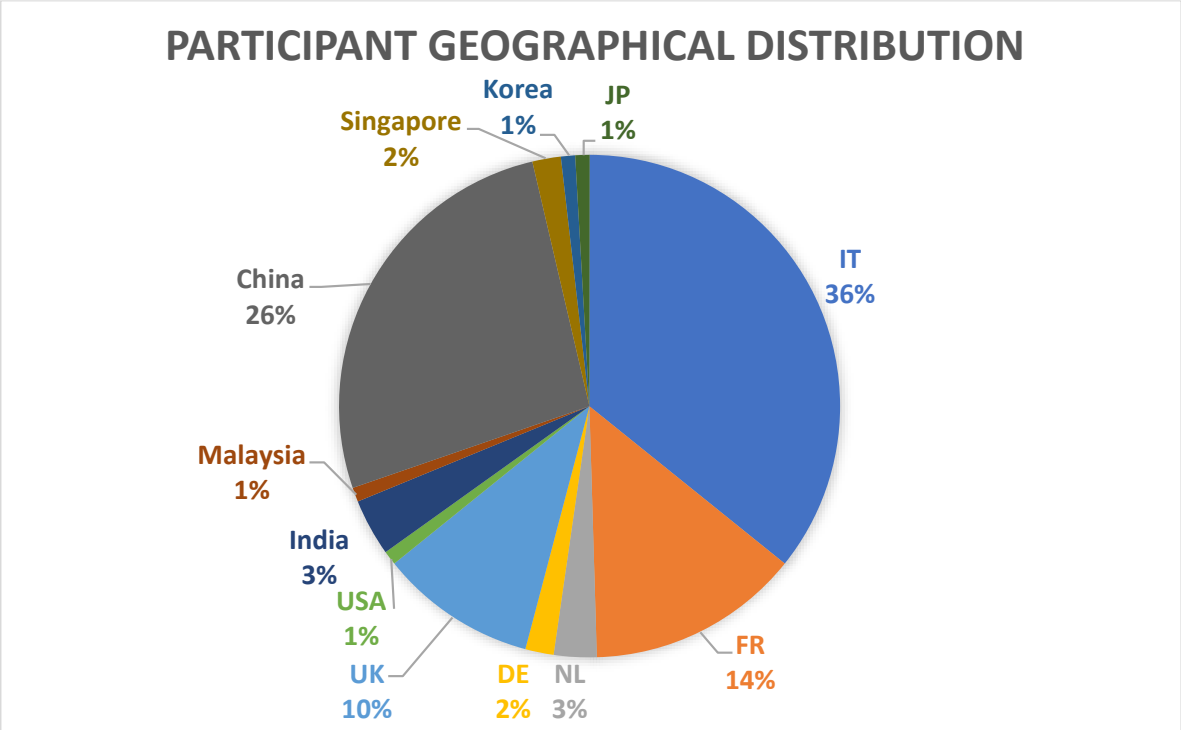
Undergraduate	13
Graduate	13
Engineer	3
Sales Manager	1
PhD	45
PostDoc	12
Researcher	17
Professor	3

The same data considered in terms of percentage is reported in the pie diagram shown below:

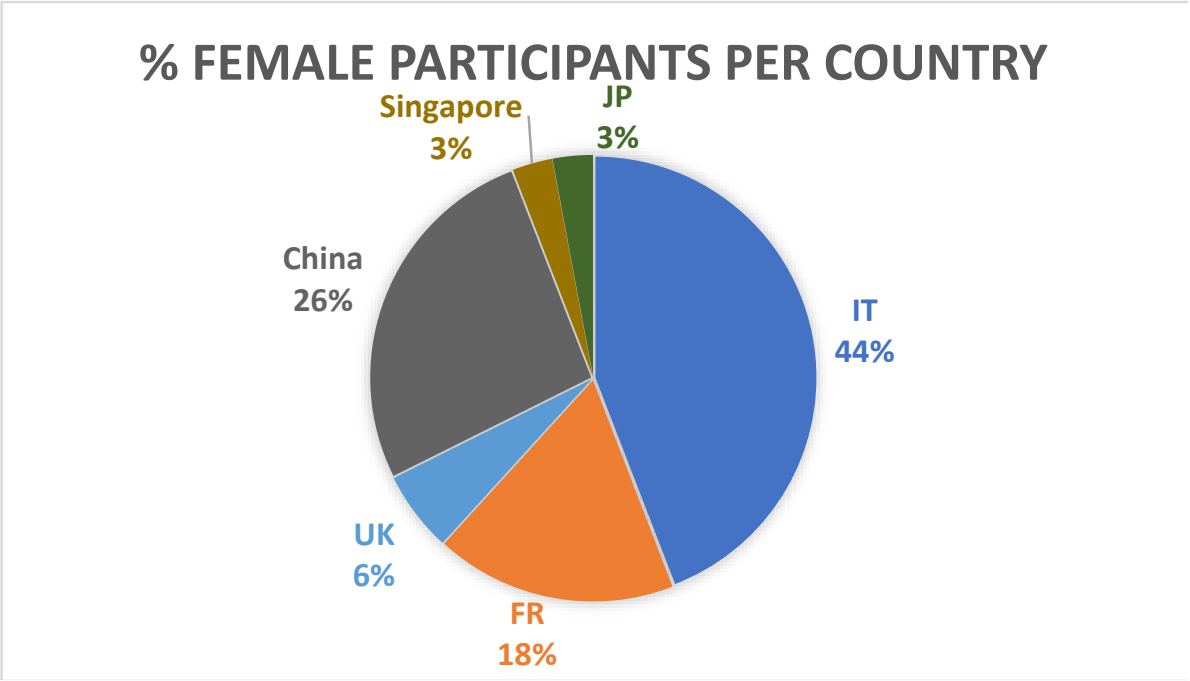


As shown clearly, we meet the scope of the event to mainly reach students and young PostDocs.

The attendees had to 27 different affiliations. The participant geographical distribution was rather broad and spread worldwide tanks to the free of charge participation and its virtual character. Nevertheless, we noticed that the time chosen was favorable to participants located in Europe and Asia. The geographical distribution pie is shown below:



In respect to gender distribution, Dr. R. Calarco as organizer together with Prof. F. Arciprete represents a 50% female representation. The female participation in the attendance is of the 31% with the distribution per country shown below:


% FEMALE PARTICIPANTS PER COUNTRY
Singapore
3%
JP
3%
China
26%
IT
44%
UK
6%
FR
18%

5 Flyer

The School was advertised at the different institutions of the consortium partners and to institutions of collaborators and colleagues of the phase change material field. As the attendance was very high, such measure resulted particularly efficient.

BeforeHand

http://www.beforehand.eu
Join on your computer or mobile app
Link to join the school meeting

FOR ENROLLEMENT PLEASE SEND AN E-MAIL TO:
raffaella.calarco@cnr.it
fabrizio.arciprete@roma2.infn.it

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6 Certificate of attendance

Below it is shown a template of the certificate of attendance that we provided to those who connected for the school seminars and attended the courses.